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N-(Biphenyl-4-carbonyl)-*N*′-(2-chlorophenyl)thiourea

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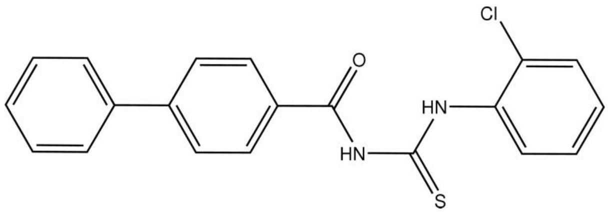
Key indicators: single-crystal X-ray study; *T* = 298 K; mean σ(C–C) = 0.005 Å; *R* factor = 0.063; *wR* factor = 0.131; data-to-parameter ratio = 13.8.

In the title compound, $C_{20}H_{15}ClN_2OS$, the benzene rings of the biphenyl group are not coplanar, indicated by a dihedral angle of 20.71 (17)°. The molecule maintains its *trans–cis* configuration with respect to the position of the biphenylcarbonyl and chlorobenzene groups relative to the thiono S atom across their C—N bonds, respectively. The central carbonyl–thiourea unit makes dihedral angles with the carbonyl benzene ring and the chlorobenzene fragment of 24.39 (13) and 61.63 (10)°, respectively. There is an intramolecular N—H···O hydrogen bond in the molecule. The molecules in the structure are packed by weak van der Waals and π–π interactions [centroid–centroid distance 3.629 (2) Å].

Related literature

Many *N*-aroyl-*N*′(chlorophenyl)thiourea compounds, such as *N*-benzoyl-*N*′-(2-chlorophenyl)thiourea (Yusof & Yamin, 2004) and *N*-pivaloyl-*N*′-(2-chlorophenyl)thiourea (Shoukat *et al.*, 2007), possess a *trans–cis* configuration with respect to the position of the carbonyl and chlorophenyl groups relative to the thiono S atom about their thiourea C—N bonds, respectively.

For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{20}H_{15}ClN_2OS$
M_r = 366.85
Monoclinic, $P2_1/n$
a = 9.2448 (14) Å
b = 7.2284 (11) Å
c = 25.934 (4) Å
β = 90.295 (3)°
V = 1733.0 (5) Å^3
Z = 4
Mo *K*α radiation
μ = 0.35 mm^{-1}
T = 298 (2) K
0.50 × 0.30 × 0.07 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.844, T_{max} = 0.975
8945 measured reflections
3219 independent reflections
1742 reflections with $I > 2\sigma(I)$
R_{int} = 0.064

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.131
S = 1.02
3219 reflections
234 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1	0.863 (12)	1.882 (18)	2.619 (4)	142 (3)

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2028).

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supplementary materials

Acta Cryst. (2007). E**63**, o3594 [**doi:10.1107/S1600536807035179**]

N-(Biphenyl-4-carbonyl)-*N*'-(2-chlorophenyl)thiourea

M. A. M. Arif and **B. M. Yamin**

Comment

Many aroylthiourea compounds reported so far are based on a benzene group. The title compound, (I), is also an aroylthiourea derivative but having a biphenyl group (Fig.1). The molecule maintains the *trans-cis* configuration with respect to the position of the biphenylcarbonyl and chlorobenzene groups about the thiono sulfur atom across their C14—N1 and C14—N2 bonds, respectively. The biphenyl fragment is not planar with C1—C6—C7—C12 and C5—C6—C7—C8 torsion angles of −18.9 (5) and −21.2 (5)° respectively. The bond lengths and angles are in normal ranges (Allen *et al.*, 1987) and close to those observed in (II) (Yusof & Yamin, 2004) and (III) (Shoukat *et al.*, 2007). The benzene C7—C12, the carbonyl-thiourea C13/O1/N1/C14/S1/N2 and the chlorobenzene Cl1/C15—C20 fragments are each planar with maximum deviation of 0.026 (3)Å for N1 atom from the least squares plane of the carbonyl-thiourea moiety. The central carbonyl-thiourea moiety makes dihedral angles with the C7—C12 benzene ring and chlorobenzene fragment of 24.39 (13) and 61.63 (10)°, respectively. There is an N2—H2A···O1 intramolecular hydrogen bond (D—H= 0.863 (12), H···A= 1.882 (18) D···A= 2.619 (4)Å and D—H···A =142 (3)°) formimg a pseudo six-membered ring [C13—N1—C14—N2—H2A···O1]. The crystal packing is stabilized by weak van der Waals and π···π interactions, between the benzene $(C7—C12)^i$ rings ((i): 1 − *x*, −*y*, −*z*) with the distance between the centroids of 3.629 (2) Å.

Experimental

A solution of 2-chloroaniline (0.63 g, 2.5 mmol) in 20 ml acetone was added dropwise to a two-necked round-bottomed flask containing an equimolar solution of biphenylcarbomoylisothiocyanate (0.60 g, 2.5 mmol) in 20 ml of acetone. The mixture was refluxed for about 3 h. The light yellow solution was filtered and allowed to evaporate at room temperature. Some colourless crystals were obtained after five days of evaporation (yield 0.71 g, 85%).

Refinement

H atoms on C were positioned geometrically with C—H 0.93, 0.96 and 0.97 Å, for aromatic, methlylene and methyl H atoms respectively, constrained to ride on their parent atoms with $U_{iso}(H)= 1.2U_{eq}(C)$. The hydrogen atom attached to the N atom were located from the difference map and refined isotropically.

Figures

Fig. 1. Molecular structure of compound, (1), with displacement ellipsoid drawn at the 50% probablity level. The dashed line indicates the intramolecular hydrogen bond.

N-(Biphenyl-4-carbonyl)-*N*'-(2-chlorophenyl)thiourea

Crystal data

$C_{20}H_{15}ClN_2OS$

$M_r = 366.85$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 9.2448$ (14) Å

$b = 7.2284$ (11) Å

$c = 25.934$ (4) Å

$\beta = 90.295$ (3)°

$V = 1733.0$ (5) Å^3

$Z = 4$

$F_{000} = 760$

$D_x = 1.406$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 993 reflections

$\theta = 1.5–26.0$°

$\mu = 0.35$ mm^{-1}

$T = 298$ (2) K

Slab, colourless

0.50 × 0.30 × 0.07 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 83.66 pixels mm^{-1}

$T = 298(2)$ K

ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2000)

$T_{min} = 0.844$, $T_{max} = 0.975$

8945 measured reflections

3219 independent reflections

1742 reflections with $I > 2\sigma(I)$

$R_{int} = 0.064$

$\theta_{max} = 26.0$°

$\theta_{min} = 1.5$°

$h = -11 \rightarrow 10$

$k = -8 \rightarrow 8$

$l = -29 \rightarrow 31$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.063$

$wR(F^2) = 0.131$

$S = 1.02$

3219 reflections

234 parameters

2 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 0.1441P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.17$ e Å^{-3}

$\Delta\rho_{min} = -0.17$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\mathrm{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	1.27749 (11)	0.44805 (15)	0.13364 (4)	0.0817 (4)
S1	0.88704 (10)	0.09939 (17)	0.21077 (4)	0.0781 (4)
O1	0.9742 (3)	0.1787 (4)	0.04062 (9)	0.0664 (8)
N1	0.8363 (3)	0.1431 (4)	0.11180 (11)	0.0503 (7)
H1A	0.7484 (15)	0.138 (5)	0.1217 (12)	0.071 (12)*
N2	1.0760 (3)	0.1311 (4)	0.13409 (11)	0.0523 (8)
H2A	1.084 (3)	0.143 (4)	0.1011 (4)	0.051 (10)*
C1	0.3650 (4)	0.3033 (5)	−0.12193 (13)	0.0567 (10)
H1B	0.4552	0.2864	−0.1370	0.068*
C2	0.2491 (4)	0.3507 (6)	−0.15248 (14)	0.0695 (11)
H2B	0.2623	0.3679	−0.1877	0.083*
C3	0.1151 (4)	0.3727 (5)	−0.13193 (15)	0.0640 (10)
H3A	0.0369	0.4040	−0.1528	0.077*
C4	0.0972 (4)	0.3481 (5)	−0.08032 (15)	0.0618 (10)
H4A	0.0062	0.3637	−0.0658	0.074*
C5	0.2130 (4)	0.3003 (5)	−0.04933 (13)	0.0548 (9)
H5A	0.1983	0.2811	−0.0143	0.066*
C6	0.3507 (3)	0.2803 (4)	−0.06939 (12)	0.0431 (8)
C7	0.4769 (3)	0.2416 (4)	−0.03535 (12)	0.0426 (8)
C8	0.4740 (4)	0.2821 (4)	0.01696 (13)	0.0502 (9)
H8A	0.3892	0.3289	0.0310	0.060*
C9	0.5914 (4)	0.2560 (5)	0.04891 (13)	0.0512 (9)
H9A	0.5839	0.2819	0.0839	0.061*
C10	0.7212 (3)	0.1910 (4)	0.02908 (12)	0.0441 (8)
C11	0.7267 (4)	0.1514 (5)	−0.02322 (13)	0.0526 (9)
H11A	0.8127	0.1087	−0.0374	0.063*
C12	0.6070 (4)	0.1741 (5)	−0.05464 (13)	0.0515 (9)
H12A	0.6133	0.1438	−0.0894	0.062*
C13	0.8543 (4)	0.1702 (5)	0.06013 (13)	0.0487 (9)
C14	0.9399 (4)	0.1239 (5)	0.15061 (12)	0.0496 (9)
C15	1.2018 (3)	0.1052 (5)	0.16435 (12)	0.0464 (9)
C16	1.3065 (4)	0.2418 (5)	0.16584 (12)	0.0517 (9)
C17	1.4339 (4)	0.2124 (7)	0.19269 (15)	0.0722 (12)

H17A	1.5049	0.3036	0.1934	0.087*
C18	1.4555 (4)	0.0495 (8)	0.21814 (15)	0.0808 (14)
H18A	1.5412	0.0305	0.2364	0.097*
C19	1.3519 (5)	−0.0868 (7)	0.21709 (14)	0.0812 (13)
H19A	1.3671	−0.1973	0.2347	0.097*
C20	1.2259 (4)	−0.0589 (6)	0.18997 (13)	0.0645 (11)
H20A	1.1562	−0.1516	0.1889	0.077*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0681 (7)	0.0663 (7)	0.1108 (9)	−0.0126 (6)	0.0092 (6)	0.0044 (7)
S1	0.0552 (6)	0.1315 (11)	0.0477 (6)	−0.0086 (6)	0.0052 (5)	−0.0061 (6)
O1	0.0459 (15)	0.096 (2)	0.0570 (16)	−0.0027 (14)	0.0110 (12)	0.0065 (14)
N1	0.0387 (18)	0.067 (2)	0.0453 (19)	−0.0106 (16)	0.0027 (15)	−0.0040 (15)
N2	0.0409 (18)	0.071 (2)	0.0447 (19)	−0.0087 (15)	0.0037 (15)	0.0036 (17)
C1	0.050 (2)	0.072 (3)	0.048 (2)	−0.0094 (19)	0.0071 (18)	−0.002 (2)
C2	0.067 (3)	0.092 (3)	0.050 (2)	−0.010 (2)	−0.005 (2)	0.006 (2)
C3	0.052 (2)	0.071 (3)	0.069 (3)	−0.004 (2)	−0.008 (2)	0.007 (2)
C4	0.049 (2)	0.067 (3)	0.069 (3)	0.0027 (19)	0.007 (2)	0.001 (2)
C5	0.057 (2)	0.053 (2)	0.055 (2)	−0.0055 (18)	0.010 (2)	0.0032 (19)
C6	0.048 (2)	0.034 (2)	0.048 (2)	−0.0089 (16)	0.0040 (17)	0.0003 (16)
C7	0.049 (2)	0.035 (2)	0.043 (2)	−0.0113 (16)	0.0084 (17)	0.0013 (16)
C8	0.046 (2)	0.052 (2)	0.052 (2)	−0.0012 (17)	0.0104 (18)	−0.0009 (19)
C9	0.055 (2)	0.055 (2)	0.043 (2)	−0.0039 (18)	0.0033 (18)	−0.0032 (18)
C10	0.049 (2)	0.039 (2)	0.043 (2)	−0.0098 (16)	0.0041 (17)	−0.0018 (17)
C11	0.049 (2)	0.055 (2)	0.054 (2)	−0.0022 (18)	0.0115 (18)	−0.0031 (19)
C12	0.053 (2)	0.054 (2)	0.048 (2)	−0.0052 (18)	0.0076 (18)	−0.0029 (18)
C13	0.052 (2)	0.046 (2)	0.048 (2)	−0.0071 (17)	0.0042 (19)	−0.0005 (17)
C14	0.049 (2)	0.051 (2)	0.049 (2)	−0.0133 (17)	0.0039 (18)	−0.0087 (18)
C15	0.040 (2)	0.055 (3)	0.044 (2)	0.0010 (18)	0.0050 (16)	−0.0039 (19)
C16	0.050 (2)	0.056 (2)	0.049 (2)	−0.0038 (19)	0.0036 (18)	−0.0089 (19)
C17	0.048 (3)	0.106 (4)	0.063 (3)	−0.013 (2)	0.004 (2)	−0.013 (3)
C18	0.050 (3)	0.137 (5)	0.056 (3)	0.013 (3)	−0.002 (2)	0.004 (3)
C19	0.069 (3)	0.112 (4)	0.062 (3)	0.016 (3)	0.009 (2)	0.025 (3)
C20	0.063 (3)	0.071 (3)	0.060 (2)	0.001 (2)	0.009 (2)	0.011 (2)

Geometric parameters (Å, °)

Cl1—C16	1.729 (4)	C7—C8	1.388 (4)
S1—C14	1.647 (3)	C7—C12	1.393 (4)
O1—C13	1.222 (3)	C8—C9	1.375 (4)
N1—C13	1.365 (4)	C8—H8A	0.9300
N1—C14	1.393 (4)	C9—C10	1.390 (4)
N1—H1A	0.855 (10)	C9—H9A	0.9300
N2—C14	1.332 (4)	C10—C11	1.387 (4)
N2—C15	1.413 (4)	C10—C13	1.475 (4)
N2—H2A	0.865 (10)	C11—C12	1.381 (4)
C1—C2	1.373 (5)	C11—H11A	0.9300

C1—C6	1.380 (4)	C12—H12A	0.9300
C1—H1B	0.9300	C15—C20	1.378 (5)
C2—C3	1.360 (5)	C15—C16	1.383 (4)
C2—H2B	0.9300	C16—C17	1.382 (5)
C3—C4	1.361 (5)	C17—C18	1.364 (5)
C3—H3A	0.9300	C17—H17A	0.9300
C4—C5	1.379 (4)	C18—C19	1.374 (6)
C4—H4A	0.9300	C18—H18A	0.9300
C5—C6	1.386 (4)	C19—C20	1.373 (5)
C5—H5A	0.9300	C19—H19A	0.9300
C6—C7	1.486 (4)	C20—H20A	0.9300

C13—N1—C14	129.6 (3)	C11—C10—C9	117.9 (3)
C13—N1—H1A	115 (2)	C11—C10—C13	118.5 (3)
C14—N1—H1A	116 (2)	C9—C10—C13	123.5 (3)
C14—N2—C15	126.4 (3)	C12—C11—C10	121.3 (3)
C14—N2—H2A	114 (2)	C12—C11—H11A	119.4
C15—N2—H2A	119 (2)	C10—C11—H11A	119.4
C2—C1—C6	121.4 (3)	C11—C12—C7	121.4 (3)
C2—C1—H1B	119.3	C11—C12—H12A	119.3
C6—C1—H1B	119.3	C7—C12—H12A	119.3
C3—C2—C1	120.8 (4)	O1—C13—N1	121.9 (3)
C3—C2—H2B	119.6	O1—C13—C10	121.6 (3)
C1—C2—H2B	119.6	N1—C13—C10	116.4 (3)
C2—C3—C4	119.0 (3)	N2—C14—N1	114.2 (3)
C2—C3—H3A	120.5	N2—C14—S1	126.5 (3)
C4—C3—H3A	120.5	N1—C14—S1	119.3 (2)
C3—C4—C5	120.5 (3)	C20—C15—C16	119.4 (3)
C3—C4—H4A	119.7	C20—C15—N2	120.8 (3)
C5—C4—H4A	119.7	C16—C15—N2	119.7 (3)
C4—C5—C6	121.3 (3)	C17—C16—C15	119.9 (4)
C4—C5—H5A	119.4	C17—C16—Cl1	120.4 (3)
C6—C5—H5A	119.4	C15—C16—Cl1	119.7 (3)
C1—C6—C5	116.8 (3)	C18—C17—C16	119.9 (4)
C1—C6—C7	122.0 (3)	C18—C17—H17A	120.0
C5—C6—C7	121.1 (3)	C16—C17—H17A	120.0
C8—C7—C12	116.5 (3)	C17—C18—C19	120.6 (4)
C8—C7—C6	121.5 (3)	C17—C18—H18A	119.7
C12—C7—C6	121.9 (3)	C19—C18—H18A	119.7
C9—C8—C7	122.7 (3)	C20—C19—C18	119.7 (4)
C9—C8—H8A	118.6	C20—C19—H19A	120.2
C7—C8—H8A	118.6	C18—C19—H19A	120.2
C8—C9—C10	120.2 (3)	C19—C20—C15	120.5 (4)
C8—C9—H9A	119.9	C19—C20—H20A	119.7
C10—C9—H9A	119.9	C15—C20—H20A	119.7

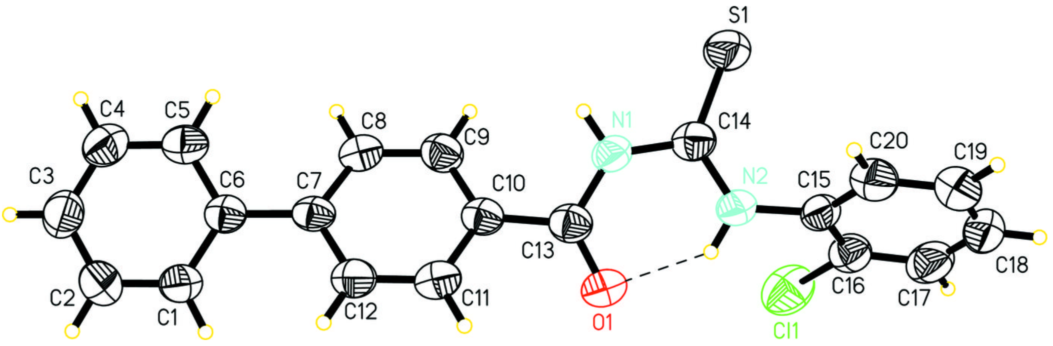
C6—C1—C2—C3	−1.4 (6)	C14—N1—C13—C10	−178.2 (3)
C1—C2—C3—C4	0.4 (6)	C11—C10—C13—O1	24.0 (5)
C2—C3—C4—C5	−0.5 (6)	C9—C10—C13—O1	−153.1 (3)
C3—C4—C5—C6	1.6 (5)	C11—C10—C13—N1	−156.7 (3)

C2—C1—C6—C5	2.4 (5)	C9—C10—C13—N1	26.2 (5)
C2—C1—C6—C7	−175.8 (3)	C15—N2—C14—N1	−176.2 (3)
C4—C5—C6—C1	−2.5 (5)	C15—N2—C14—S1	5.1 (5)
C4—C5—C6—C7	175.7 (3)	C13—N1—C14—N2	−0.9 (5)
C1—C6—C7—C8	156.9 (3)	C13—N1—C14—S1	177.9 (3)
C5—C6—C7—C8	−21.2 (5)	C14—N2—C15—C20	60.3 (5)
C1—C6—C7—C12	−18.9 (5)	C14—N2—C15—C16	−123.6 (4)
C5—C6—C7—C12	163.0 (3)	C20—C15—C16—C17	0.3 (5)
C12—C7—C8—C9	−0.8 (5)	N2—C15—C16—C17	−175.8 (3)
C6—C7—C8—C9	−176.8 (3)	C20—C15—C16—Cl1	179.8 (2)
C7—C8—C9—C10	1.7 (5)	N2—C15—C16—Cl1	3.7 (4)
C8—C9—C10—C11	−1.0 (5)	C15—C16—C17—C18	−0.7 (5)
C8—C9—C10—C13	176.1 (3)	Cl1—C16—C17—C18	179.8 (3)
C9—C10—C11—C12	−0.5 (5)	C16—C17—C18—C19	0.4 (6)
C13—C10—C11—C12	−177.8 (3)	C17—C18—C19—C20	0.3 (6)
C10—C11—C12—C7	1.4 (5)	C18—C19—C20—C15	−0.8 (6)
C8—C7—C12—C11	−0.7 (5)	C16—C15—C20—C19	0.5 (5)
C6—C7—C12—C11	175.3 (3)	N2—C15—C20—C19	176.5 (3)
C14—N1—C13—O1	1.1 (6)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O1	0.863 (12)	1.882 (18)	2.619 (4)	142 (3)

Fig. 1


S1
C4
C5
C8
C9
N1
C14
C20
C19
C3
C6
C7
C10
N2
C15
C18
C13
C16
C2
C1
C12
C11
O1
C17
Cl1